Non-Perturbative Determination of the Shell Model Effective Interaction

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Limits of nuclear existence

Towards a unified description of the nucleus

Coupled Cluster approach
GFMC formalism

Ab initio few-body calculations

No-Core Shell Model

Density Functional Theory
Selfconsistent Mean Field

r-process
OUTLINE

I. Overview of the *Ab Initio* Shell Model with a Core Approach

II. Results:
   a.) General sd-shell
   b.) Fluorine isotopes

III. Summary/Outlook
I. Overview of the *Ab Initio* Shell Model with a Core Approach
From few-body to many-body

Using the NCSM to calculate the shell model input

**Ab initio**
No Core Shell Model

Realistic NN & NNN forces

Effective interactions in cluster approximation

Diagonalization of many-body Hamiltonian

Core Shell Model

effective interactions for valence nucleons

Diagonalization of the Hamiltonian for valence nucleons

Many-body experimental data
Effective interaction in a projected model space

\[ H \Psi_\alpha = E_\alpha \Psi_\alpha \]

where

\[ H = \sum_{i=1}^{A} t_i + \sum_{i \leq j}^{A} v_{ij}. \]

\[ \mathcal{H} \Phi_\beta = E_\beta \Phi_\beta \]

\[ \Phi_\beta = P \Psi_\beta \]

\( P \) is a projection operator from \( S \) into \( S \)

\[ < \Phi_\gamma | \Phi_\beta > = \delta_{\gamma \beta} \]

\[ \mathcal{H} = \sum_{\beta \in S} |\Phi_\beta > E_\beta < \Phi_\beta| \]
\[ N_a + N_b \leq N_{\text{max}} + 2 \]

\[ Q_1 \]

\[ Q_2 = P_1 - P_2 \]
Ab-initio shell model with a core

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We construct effective two- and three-body Hamiltonians for the $p$-shell by performing $12\hbar\Omega$ ab initio no-core shell model (NCSM) calculations for $A = 6$ and 7 nuclei and explicitly projecting the many-body Hamiltonians onto the $0\hbar\Omega$ space. We then separate these effective Hamiltonians into inert core, one- and two-body contributions (also three-body for $A = 7$) and analyze the systematic behavior of these different parts as a function of the mass number $A$ and size of the NCSM basis space. The role of effective three- and higher-body interactions for $A > 6$ is investigated and discussed.

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FORMALISM

1. Perform a large basis NCSM for a core + 2N system, e.g., $^{18}\text{F}$.

2. Use Okubo-Lee-Suzuki transformation to project these results into a single major shell to obtain effective 2-body matrix elements.

3. Separate these 2-body matrix elements into a core term, single-particle energies and residual 2-body interactions, i.e., the standard input for a normal Shell Model calculation.

4. Use these values for performing SM calculations in that shell.
II. Results: a.) sd-shell nuclei
Ab initio effective interactions for sd-shell valence nucleons

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(Dated: February 3, 2015)

We perform ab initio no core shell model calculations for \(A = 18\) and \(19\) nuclei in a \(4\hbar\Omega\), or \(N_{\text{max}} = 4\), model space using the effective JISP16 and chiral N3LO nucleon-nucleon potentials and transform the many-body effective Hamiltonians into the \(0\hbar\Omega\) model space to construct the \(A\)-body effective Hamiltonians in the \(sd\)-shell. We separate the \(A\)-body effective Hamiltonians with \(A = 18\) and \(A = 19\) into inert core, one- and two-body components. Then, we use these core, one- and two-body components to perform standard shell model calculations for the \(A = 18\) and \(A = 19\) systems with valence nucleons restricted to the \(sd\)-shell. Finally, we compare the standard shell model results in the \(0\hbar\Omega\) model space with the exact no core shell model results in the \(4\hbar\Omega\) model space for the \(A = 18\) and \(A = 19\) systems and find good agreement.

ArXiv: Nucl-th 1502.00700
Empirical Single-Particle Energies

\[ E_{0d_{3/2}} = 0.0 \text{ MeV} \]
\[ E_{15s_{1/2}} = 0.87 \text{ MeV} \]
\[ E_{0d_{5/2}} = 5.08 \text{ MeV} \]

\[
\mathcal{H}_{eff}^{sd}(P_{\pi\nu})^{sd} = \left\{ \sum_{i} \epsilon_{i} + \tilde{V}_{eff}^{sd} \right\}(P_{\pi\nu})^{sd}
\]

\[
[H_0 + \tilde{V}_{eff}^{sd}](P_{\pi\nu})^{sd} = E^{sd}(P_{\pi\nu})^{sd}
\]
Input: The results of $N_{\text{max}} = 4$ and $hw = 14$ MeV NCSM calculations

**TABLE II:** Proton and neutron single-particle energies (in MeV) for JISP16 effective interaction obtained for the mass of $A = 18$ and $A = 19$.

<table>
<thead>
<tr>
<th>$j_i$</th>
<th>$\frac{1}{2}$</th>
<th>$\frac{5}{2}$</th>
<th>$\frac{3}{2}$</th>
<th>$\frac{1}{2}$</th>
<th>$\frac{5}{2}$</th>
<th>$\frac{3}{2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_{j_i}^{p}$</td>
<td>-3.068</td>
<td>-2.270</td>
<td>6.262</td>
<td>-3.044</td>
<td>-2.248</td>
<td>6.289</td>
</tr>
<tr>
<td>$e_{j_i}^{n}$</td>
<td>0.603</td>
<td>1.398</td>
<td>9.748</td>
<td>0.627</td>
<td>1.419</td>
<td>9.774</td>
</tr>
</tbody>
</table>

**TABLE III:** Proton and neutron single-particle energies (in MeV) for chiral N3LO effective interaction obtained for the mass of $A = 18$ and $A = 19$.

<table>
<thead>
<tr>
<th>$j_i$</th>
<th>$\frac{1}{2}$</th>
<th>$\frac{5}{2}$</th>
<th>$\frac{3}{2}$</th>
<th>$\frac{1}{2}$</th>
<th>$\frac{5}{2}$</th>
<th>$\frac{3}{2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$e_{j_i}^{n}$</td>
<td>-3.638</td>
<td>-3.042</td>
<td>3.763</td>
<td>-3.625</td>
<td>-3.031</td>
<td>3.770</td>
</tr>
<tr>
<td>$e_{j_i}^{p}$</td>
<td>0.044</td>
<td>0.690</td>
<td>7.299</td>
<td>0.057</td>
<td>0.700</td>
<td>7.307</td>
</tr>
</tbody>
</table>

**Coupled Cluster, $E_{\text{core}}$:**
-130.462

**Idaho NN N3LO + 3N N2LO**

**IM-SRG, $E_{\text{core}}$:**
-130.132

**Idaho NN N3LO + 3N N2LO**

for G.R. Jansen et al. PRL 113, 142502 (2014)

-130.056

for H. Hergert private comm.

-129.637
No-Core Shell-Model Approach

Next, add CM harmonic-oscillator Hamiltonian

\[ H_{CM}^{HO} = \frac{\vec{P}^2}{2Am} + \frac{1}{2} Am\Omega^2 \vec{R}^2; \quad \vec{R} = \frac{1}{A} \sum_{i=1}^{A} \vec{r}_i, \quad \vec{P} = Am\dot{\vec{R}} \]

To \( H_A \), yielding

\[ H_A^{\Omega} = \sum_{i=1}^{A} \left[ \frac{\vec{p}_i^2}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^2 \right] + \sum_{i<j=1}^{A} \left[ V_{NN}(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right] \]

Defines a basis (i.e. \( HO \)) for evaluating \( V_{ij} \)
PRELIMINARY RESULT

RMS: 0.000128
II. Results: b) Fluorine isotopes
Effects of 3NFs on single-particle energies vs effects of 3NFs on TBMEs

(16 \times 15)/2 = 120 terms in the sum over core nucleons

16 terms in the sum over core nucleons
Survey of the Fluorine isotopes

1. Calculate the Fluorine isotopes using the same set of effective TBMEs, which are very weakly A-dependent, e.g., those determined from the N3LO NN interaction, to test how well they reproduce data trends.

2. Approximate the effect of 3NFs by replacing our theoretical single-particle energies with the theoretical ones obtained in the IM-SRG calculations of S.R. Stroberg et al.*

3. Compare our results for the F isotopes with those obtained with the IM-SRG approach* using an EFT N3LO NN plus N2LO NNN interaction and with experiment.

\textbf{PRELIMINARY RESULT}

\begin{figure}
\centering
\begin{tikzpicture}
\begin{axis}[
    title={$^{17}\text{F}$},
    xlabel={\textbf{\(E\) (MeV)}},
    ylabel={},
    xmin=0, xmax=10,
    ymin=0, ymax=10,
    axis x line=middle,
    axis y line=middle,
    axis line style={-},
    tick align=outside,
    xtick={0,2,4,6,8,10},
    ytick={0,2,4,6,8,10},
    xticklabels={\(5/2^+\), \(5/2^+\), \(5/2^+\), \(5/2^+\), \(5/2^+\), \(5/2^+\)},
    yticklabels={},
    xticklabel style={text width=1cm, align=center},
    yticklabel style={},
    xticklabel style={font=\scriptsize},
    yticklabel style={font=\scriptsize},
    xticklabel style={text width=1cm, align=center},
    yticklabel style={font=\scriptsize},
    xticklabel style={text width=1cm, align=center},
    yticklabel style={font=\scriptsize},
    xticklabel style={text width=1cm, align=center},
    yticklabel style={font=\scriptsize},
]
\addplot[red, line width=1.0pt, mark=none]
coordinates{
    (0,10) (2,8) (4,6) (6,4) (8,2) (10,0)
};
\addplot[red, line width=1.0pt, mark=none]
coordinates{
    (0,8) (2,6) (4,4) (6,2) (8,0)
};
\addplot[red, line width=1.0pt, mark=none]
coordinates{
    (0,6) (2,4) (4,2) (6,0)
};
\addplot[red, line width=1.0pt, mark=none]
coordinates{
    (0,4) (2,2) (4,0)
};
\addplot[red, line width=1.0pt, mark=none]
coordinates{
    (0,2) (2,0)
};
\end{axis}
\end{tikzpicture}
\end{figure}
* S.R. Stroberg, et al., arXiv Nucl-th 1511.02802
SUMMARY AND OUTLOOK

1. The interactions and approaches used in this study reproduced the gross trends and features of the experimental data for the Fluorine isotopes studied so far.

2. Replacing our theoretical s.p. energies with those obtained in the IM-SRG calculations of Stroberg et al. to approximate the effects of a NNN interaction, in general, improved the agreement with experiment.

3. The overall, reasonable agreement with experiment obtained using the IM-SRG approach with an EFT N3LO NN and N2LO NNN suggests that the trends in our results should continue to improve as we improve the interactions used and increase the size of our model space for our NCSM calculations.

4. The current results support the hypothesis that a single A-independent set of effective TBMEs can explain the trends in the F isotopes.

OUTLOOK: Extend our calculations to other nuclei in the sd-shell to study charge dependence. Also study the hw dependence of our results.